

Quantum critical dynamics of a magnetic impurity in a semiconducting host

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We have investigated the finite temperature dynamics of the singlet to doublet continuous quantum phase transition in the gapped Anderson impurity model using hybridization expansion continuous time quantum Monte Carlo. Using the self-energy and the longitudinal static susceptibility, we obtain a phase diagram in the temperature-gap plane. The separatrix between the low temperature local moment phase and the high temperature generalized Fermi liquid phase of this phase diagram is shown to be the lower bound of the critical scaling region of the zero gap quantum critical point of interacting type. We have computed the nuclear magnetic spin-lattice relaxation rate, the Knight shift and the Korringa ratio, which show strong deviations for any non-zero gap from the corresponding quantities in the gapless Kondo screened impurity case.

Introduction.—The screening of a magnetic impurity by conduction electrons embodies the Kondo effect[1, 2]; a quantum many body phenomenon that arises in dilute metallic alloys and mesoscopic quantum dot systems, and is well studied theoretically and experimentally. A closely related problem, that remains to be fully understood, is that of dilute magnetic impurities in a semiconducting bath, in particular their finite temperature dynamics. This problem is of direct relevance to conventional superconductors[3, 4], valence fluctuating insulators[5, 6] and dilute magnetic semiconductors[7, 8]. Theoretical investigations of this problem have focused on the gapped Anderson impurity model (GAIM), which describes a correlated impurity coupled to a bath of conduction electrons whose density of states has a hard gap (δ) at the Fermi-level.

The GAIM has been investigated using several analytical and numerically exact methods[9–16]. Early results generated a debate about the ground state of the model, namely about the minimum gap[9–11] required to screen the impurity local moment completely at $T = 0$. A consensus has now been reached through numerical renormalization group (NRG)[12, 13] and local moment approach (LMA)[15, 16] results that in the symmetric case, the boundary quantum phase transition from a Fermi liquid singlet to a local moment doublet ground state occurs at a zero critical gap, i.e $\delta_c = 0$. In particular, the LMA yields a closed scaling form[15] for the single particle spectral function. Further, the authors found that a Kondo resonance like feature survives[15] only for $\delta \lesssim T_K$, which was confirmed by recent NRG calculations[13]. In a separate work, the authors proved a number of exact results using self-consistent perturbation theory to all orders[16], including e.g. that the ph-symmetric point of the GAIM is necessarily a non-Fermi liquid local moment phase, for all nonzero gaps.

Thus, a quantum critical point (QCP) at $\delta_c = 0$

in the symmetric GAIM has been established beyond doubt. The study of critical properties and establishing the critical region for boundary quantum phase transitions, which can occur in variants of impurity Kondo models[17–21], is one of the current research interests in condensed matter physics. In this context, the finite temperature critical region and dynamics of the GAIM have not been investigated. Presently, QCPs are classified as interacting or non-interacting type based on the presence or absence respectively of ω/T scaling in the critical region[22–24]. For the QCP in the GAIM, such an identification has not been carried out. In this work, we have studied the particle-hole symmetric case of the GAIM using the hybridization expansion version of the continuous time quantum Monte-Carlo (CTQMC)[25]. A crossover in single-particle dynamics from a low temperature local moment phase to a high temperature generalized Fermi liquid phase is used to establish a phase diagram of the GAIM in the temperature vs. gap plane. The loci of such crossovers in the phase diagram is shown, through an ω/T scaling of the dynamical susceptibility, to be the lower bound of the critical scaling region of the $\delta_c = 0$ *interacting type* QCP. Finally, the magnetic relaxation rate, the Knight shift and the Korringa ratio are shown to exhibit highly anomalous behaviour for all non-zero gaps.

Model and Formalism.—The generic Anderson model that describes a quantum impurity coupled to a bath of conduction electrons is given by

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + V \sum_{k\sigma} (c_{k\sigma}^\dagger d_\sigma + h.c.) + \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow},$$

where ϵ_k is the host dispersion and V is the hybridization which couples the impurity to the bath. ϵ_d is the orbital energy for the non-dispersive local level and U is the energy cost for double occupancy of the impurity. The bath Green's function in the Matsubara frequency space can

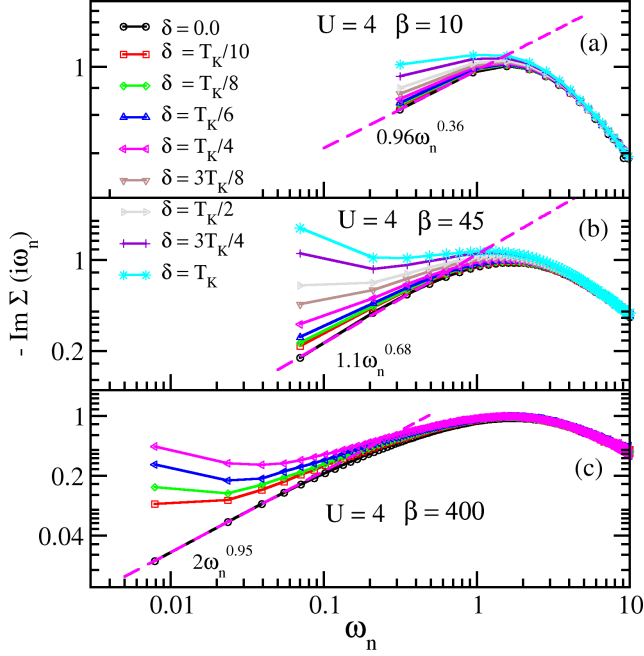


FIG. 1. (color online) Imaginary part of the Matsubara frequency self energy for a range of values of the gap in the conduction bath density of states at (a) $\beta = 10$, (b) $\beta = 45$ and (c) $\beta = 400$ with $U = 4.0$ and $V = 1.0$. The dashed line is a power law fit to the low frequency limit of the gapless case.

be written as $\mathcal{G}^0(i\omega_n) = [i\omega_n - \epsilon_d - \Delta(i\omega_n)]^{-1}$, where $\Delta(i\omega_n)$ is the hybridization function. For the GAIM, this is given by

$$\Delta(i\omega_n) = -\frac{iV^2}{D - \delta} \left[\tan^{-1} \left(\frac{D}{\omega_n} \right) - \tan^{-1} \left(\frac{\delta}{\omega_n} \right) \right], \quad (1)$$

which corresponds to a flat density of states with half-bandwidth D and a gap of 2δ at the Fermi level. We employ the hybridization expansion CTQMC[25] to measure the dynamical quantities such as single and two particle Green's functions. The hybridization expansion CTQMC method yields data on the Matsubara axis. The maximum entropy method[26] is used subsequently to obtain the real frequency dynamical spin susceptibility.

Results and discussion.— The critical gap for the level crossing transition, from a singlet Fermi liquid ground state to a doublet, is zero in the symmetric case [12, 15]. Hence at $T = 0$, we expect a local moment ground state for any non-zero δ . However, it is known from $T = 0$ LMA studies [15] that, although the low frequency single-particle spectrum of the gapped case is very different from that of the $\delta = 0$ case, the high frequency ($\omega/T_K \gg \delta/T_K$) dynamics of the gapped system is identical to that of the gapless case. Such a crossover in the $T = 0$ frequency dependence must manifest in a similar crossover in the temperature dependence. Hence, for any finite gap, the system is expected to cross over from a

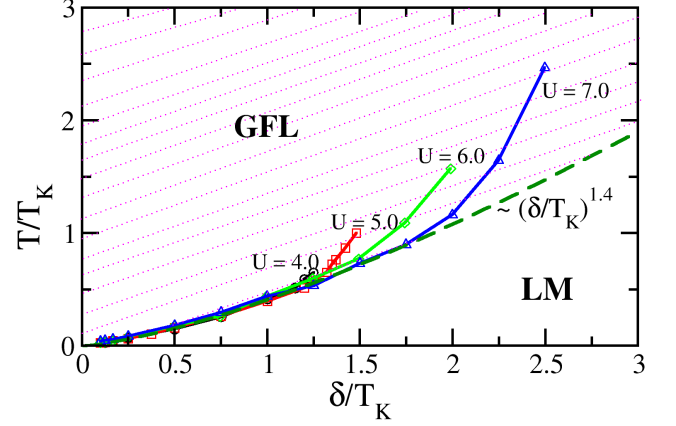


FIG. 2. (color online) A phase diagram in the T/T_K - δ/T_K plane for various U values. The shaded region is the generalized Fermi liquid (GFL) while the unshaded one is the local moment (LM) region. The dashed line is the extrapolated, asymptotic strong coupling separatrix between the GFL and LM phases.

local moment (LM) state to a generalized Fermi liquid (GFL) with increasing temperature. We now explore the finite temperature single- and two-particle quantities in the GIAM to ascertain the existence and manifestation of such an LM to GFL crossover.

The imaginary part of the self-energy is shown in Fig. 1 for various gap values and decreasing temperature (from top to bottom) for a fixed interaction strength, $U = 4$. A low frequency power law is observed in the gapless case at all temperatures, the exponent of which approaches unity as $T \rightarrow 0$. This is characteristic of Fermi liquid formation in the $\delta = 0$ case. For the $\delta > 0$ cases, although at the lowest frequencies, the $-\text{Im } \Sigma(i\omega_n)$ deviates from the power law form of the gapless case, it merges with the latter at higher ω_n . Furthermore, Fig. 1 shows that for lower gaps, the deviation from the gapless case occurs at lower temperatures. The temperature scale at which this change in the ω_n dependence (from a power law form for $\delta = 0$ to an upturn followed by a power law for any $\delta > 0$) occurs marks the crossover from a GFL to LM state and is denoted by $T_{co}(\delta, U)$. We have determined the locus of such crossover temperatures (see the SI[27] for details of the procedure) as a function of gap values for a given U and used it to construct a ‘phase diagram’ in the $T/T_K - \delta/T_K$ plane which is shown in Fig. 2.

In Fig. 2 the region above the loci (for each U) represents the GFL, while the region below is the LM state. The universal, strong coupling asymptotic locus of the crossover points is the dashed line in Fig. 2, which follows a form $T_{co} = a(\delta/T_K)^b$ with $a \sim \mathcal{O}(1)$ and $b \sim 1.4$. In the limit of vanishing gap, the crossover temperature, $T_{co} \rightarrow 0$. This corroborates the result from earlier investigations [12, 15] that the critical gap for a local moment ground state is zero in the symmetric case.

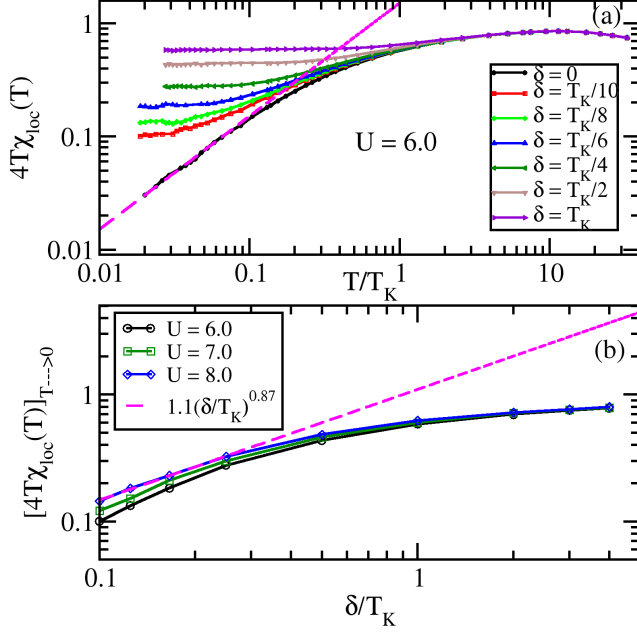


FIG. 3. (color online) (a) The product of temperature and the local static spin susceptibility ($4T\chi_{loc}(T)$) as a function of T/T_K for a range of gap values at $U = 6.0$. The dashed line is a linear fit to the gapless case. (b) The $T \rightarrow 0$ residual moment on the impurity for different U values as a function of gap. The brown dashed line is a power law fit to the small gap region of the $U = 8.0$ data.

For the gapless case ($\delta=0$), the local static spin susceptibility, namely; $\chi_{loc}(T) = \int_0^\beta d\tau \langle S_z(\tau) S_z(0) \rangle$ is known[28] to be temperature-independent for $T \ll T_K$, which represents Pauli-paramagnetic behaviour. Such behaviour indicates a complete screening of the local moment. Nozieres proposed[29] an exhaustion argument for heavy fermion systems, wherein one of the assumptions was that only those conduction electrons within an interval of $k_B T_K$ of the chemical potential are involved in the screening. However, it is now established[30] that such an assumption is unjustified. The screening process involves electrons from infrared scales all the way to logarithmically high energy scales. Thus, with a gap in the vicinity of the chemical potential, we should expect that while the screening process *will* occur, the moment will not be completely screened. Indeed, this is seen in the upper panel of Fig. 3 where we show $4T\chi_{loc}(T)$ for various gap fractions ($0.1 \leq \delta/T_K \leq 1$) as a function of temperature for a fixed $U = 6.0$. The gapless case (black symbols) shows a linear dependence (dashed line) as expected. However it must be noted that the linearity extends only up to about $T/T_K \sim 0.1$. For any finite gap, it is seen that the low temperature $T\chi_{loc}(T)$ becomes flat indicating an unscreened moment, m given by $\lim_{T \rightarrow 0} (4T\chi_{loc}(T)) = m^2$. A higher gap would lead to a lesser number of conduction states available for screening, hence the limiting zero

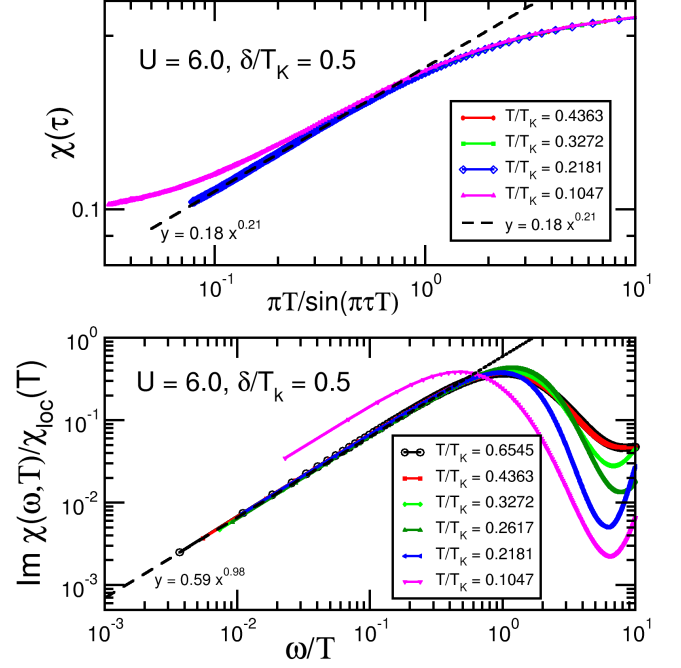


FIG. 4. (color online) Dynamical susceptibility scaling collapse: (a) $\chi(\tau)$ vs $\pi T / \sin(\pi \tau T)$, (b) $\frac{\text{Im} \chi(\omega)}{\chi_{loc}(T)}$ vs. ω/T for various temperature fractions with $U = 6.0$ and $\delta/T_K = 0.5$. The dashed lines in both the panels are power law fits.

temperature value of m must increase with increasing δ . This is shown in the lower panel of Fig. 3, where the square of the moment vs δ/T_K is shown for three different U values. A fit to the lower gap values indicates a power law dependence of m^2 on δ/T_K with the exponent ~ 0.9 . We also note that, even with a large gap of $4T_K$, only about three-fourths of the moment is unscreened, hence states from non-universal scales are involved in the Kondo screening of the magnetic moment.

Since the critical gap for the quantum phase transition from a singlet to a doublet ground state[17] is $\delta_c = 0$, and the transition is continuous, we can expect a finite temperature critical scaling region, characterized by an ω/T scaling[18] for real frequency quantities. It has been shown through boundary conformal field theory arguments that such a scaling manifests as a $\pi T / \sin(\pi \tau T)$ scaling for imaginary time quantities[18–20]. In Fig. 4, we show the susceptibility $\chi(\tau)$ computed for $U = 6$ and $\delta/T_K = 1/2$ as a function of $\pi T / \sin(\pi \tau T)$ for various temperatures. A scaling collapse is evident for temperatures $T/T_K \gtrsim 0.218$, while for lower T/T_K , a deviation from the power law scaling is observed. In the lower panel, a similar universal scaling collapse of the real frequency susceptibility (obtained through the maximum entropy method; see SI for details[27]) is observed when plotted as a function of ω/T . Such scaling behaviour has been observed previously in the pseudogap Anderson [18] and Bose-Fermi Kondo models[31]. We note that the

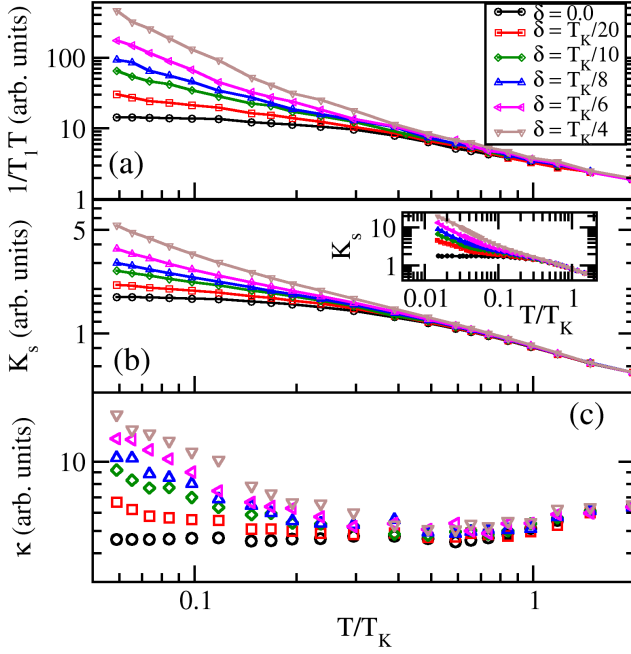


FIG. 5. (a) Magnetic relaxation rate, (b) Knight shift and (c) Korringa ratio as a function of temperature for various gap values and $U = 4.0$.

self-energy and static susceptibility show a crossover from local moment like behaviour to generalized Fermi liquid behaviour at precisely the temperature above which the scaling collapse is observed (see Fig. 1 and 2). We have verified that the same holds for other gaps as well (see figures 2 and 3 of SI[27]). Thus the shaded region of the finite temperature ‘phase diagram’ shown in Fig. 2 is in fact the critical scaling region (or the ‘fan’) of the $\delta_c = 0$ quantum critical point.

The dynamical susceptibility ($\chi(\omega, T) = \chi'(\omega, T) + i\chi''(\omega, T)$) may be used directly to calculate experimentally measurable observables such as the nuclear spin-lattice relaxation rate ($1/(T_1 T)$), Knight shift (K_s) and Korringa ratio (κ) (expressions provided in the SI[27]) [26, 32]. These three observables have been computed for various gap values and a fixed interaction strength ($U = 4$) and are shown in fig. 5 as a function of T/T_K . The singlet ground state in the gapless case implies that the relaxation mechanisms for the probe nuclear spin (e.g. ^{63}Cu) due to the impurity spin (e.g. Fe) fluctuations would be suppressed sharply as the temperature drops below the Kondo scale. Thus the relaxation time scale should diverge with decreasing temperature. The result shown in the top panel of Fig. 5 is in line with the expectations[14]. For the gapless case, where the $1/T_1 T$ saturates as $T \rightarrow 0$ implying that $T_1 \rightarrow \infty$. As seen from Fig. 3, the residual moment is finite for any non-zero gap, and moreover the magnitude of the moment increases with increasing gap as $\sim (\delta/T_K)^{0.87}$. This would then imply that the coupling between the probe nuclear spin and

the impurity moment would remain finite even as $T \rightarrow 0$. For all $\delta \gtrsim T_K/10$, we find that the $1/(T_1 T) \sim T^{-\alpha}$ with $\alpha > 1$ implying that $T_1 \sim T^{\alpha-1}$ and hence vanishes as $T \rightarrow 0$. However for $\delta = T_K/20$, we find that $\alpha \sim 0.67$, implying that T_1 diverges even though a residual moment exists. A diverging T_1 for a finite gap is surprising, and the origin of such a result is most likely that we need to go to even lower temperatures for smaller values of the gap to see the ground state behaviour. Nevertheless, the relaxation rate $1/(T_1 T)$ does diverge for any finite gap, and is hence consistent with the critical gap being zero in the symmetric case.

The Knight shift is proportional to the static susceptibility, $\chi_{loc}(T)$. Hence, at temperatures below the Kondo scale in the gapless case, the K_s should saturate, which is indeed seen in the middle panel of Fig. 5. For any non-zero gap, the ground state being a doublet should yield a $1/T$ behaviour. For the higher gaps, the $1/T$ is clearly seen while for the lower gaps, much lower temperatures ($T \ll \delta$) need to be accessed to see such behaviour (see inset of the middle panel). Shiba has considered the gapless Anderson impurity model[33] and has proved to all orders in perturbation theory that the Korringa ratio (κ) must be a constant as $T \rightarrow 0$. The bottom panel of Fig. 5 confirms this, while showing that the κ diverges with decreasing temperature for any finite gap in the host.

In the present work, the manifestation of the zero gap quantum critical point in a precisely determined finite temperature region has been demonstrated through a striking scaling collapse of the dynamical susceptibility. We have also shown that this critical scaling region is characterized by anomalous behaviour of various single-particle and two-particle static and dynamical quantities. Based on dynamical spin susceptibility scaling as a function of ω/T , we can classify the zero gap quantum critical point as an interacting type QCP. The gapped Anderson impurity model is believed to be the appropriate model for many material systems, such as dilute magnetic semiconductors and conventional superconductors. It could also be of potential relevance for lattice systems, where within the dynamical mean field theory framework, a gap could arise in the hybridization of the self-consistently determined host. Our study yields an insight into the region and extent of the influence of the zero gap quantum critical point on the finite temperature properties and hence could prove to be important for the understanding of such systems.

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